NATIONAL ENERGY TECHNOLOGY LABORATORY

NETL Modular Framework for Design & Optimization of Carbon Capture Systems

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U.S. DEPARTMENT OF ENERGY

Outline

- Motivation – CO_2 and Water
- Modular Framework – Design & Optimization
- Model details
  - PC Plant
  - MEA system
  - Compression system
- Results & Discussion
  - Power generation
  - Capital cost
  - Water use
- CCSI – Accelerating Process Scale Up

DOE/NETL Goals: CO_2 Capture

Minimum CO_2 Captured	Maximum Increase in COE
90%	30% for PC
	10% for IGCC

DOE/NETL Goals: Freshwater Minimization

- **Short-term goals (ready for commercial demonstration by 2015)**
  - Reduce freshwater withdrawal and consumption by > 50% for thermoelectric power plants equipped with wet recirculating cooling technology
  - Levelized cost savings > 25% compared to state-of-the-art dry cooling
- **Long-term goals (ready for commercial demonstration by 2020)**
  - Reduce freshwater withdrawal and consumption by > 70% for thermoelectric power plants equipped with wet recirculating cooling technology
  - Levelized cost savings > 50% compared to state-of-the-art dry cooling

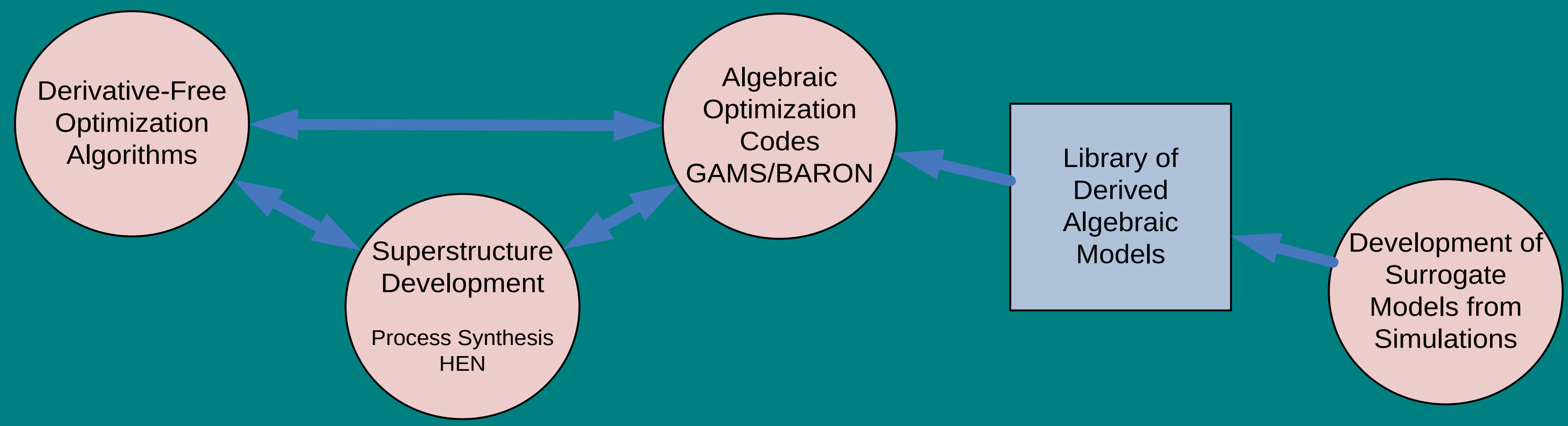
Challenges

- Large-scale problem
  - 2 billion tons CO_2 from coal by 2020 in US
  - Flue gas: 5 million lb/hr for 550MW PC plant

- No existing economical solution
- No framework for developing & evaluating <u>optimized</u> designs
- Difficulty re-using existing models/simulations
- Inconsistent assumptions & evaluation methods

- Approach
  - Process synthesis, design & optimization
    - Process integration
    - Nonlinear interactions across units/subsystems
    - Simulation-based optimization
  - Multi-criteria decision-making tools
    - Include water resource considerations

Modular Framework for Design & Optimization



Existing Plants Modules

- *Combustion system*
- *Feed water heater*
- *Boiler*
- *Economizer*
- *Superheater*
- *Steam turbines*
- *Condensers*
- *FGD*

Post-Combustion Carbon Capture Modules

- ***Amine systems***
- *Chemical looping*
- ***Solid sorbents***
- ***Adsorption***
- ***Oxycombustion***
- ***Membranes***
- *Absorption (other)*
- *Ionic liquids*
- ***Compression***

IGCC Modules

- *Feed system*
- *Gasifier*
- *Boiler*
- *Gas cleanup*
- *Shift reactor*
- *Gas turbine*
- *HRSG*
- *Steam turbines*
- *Condensers*

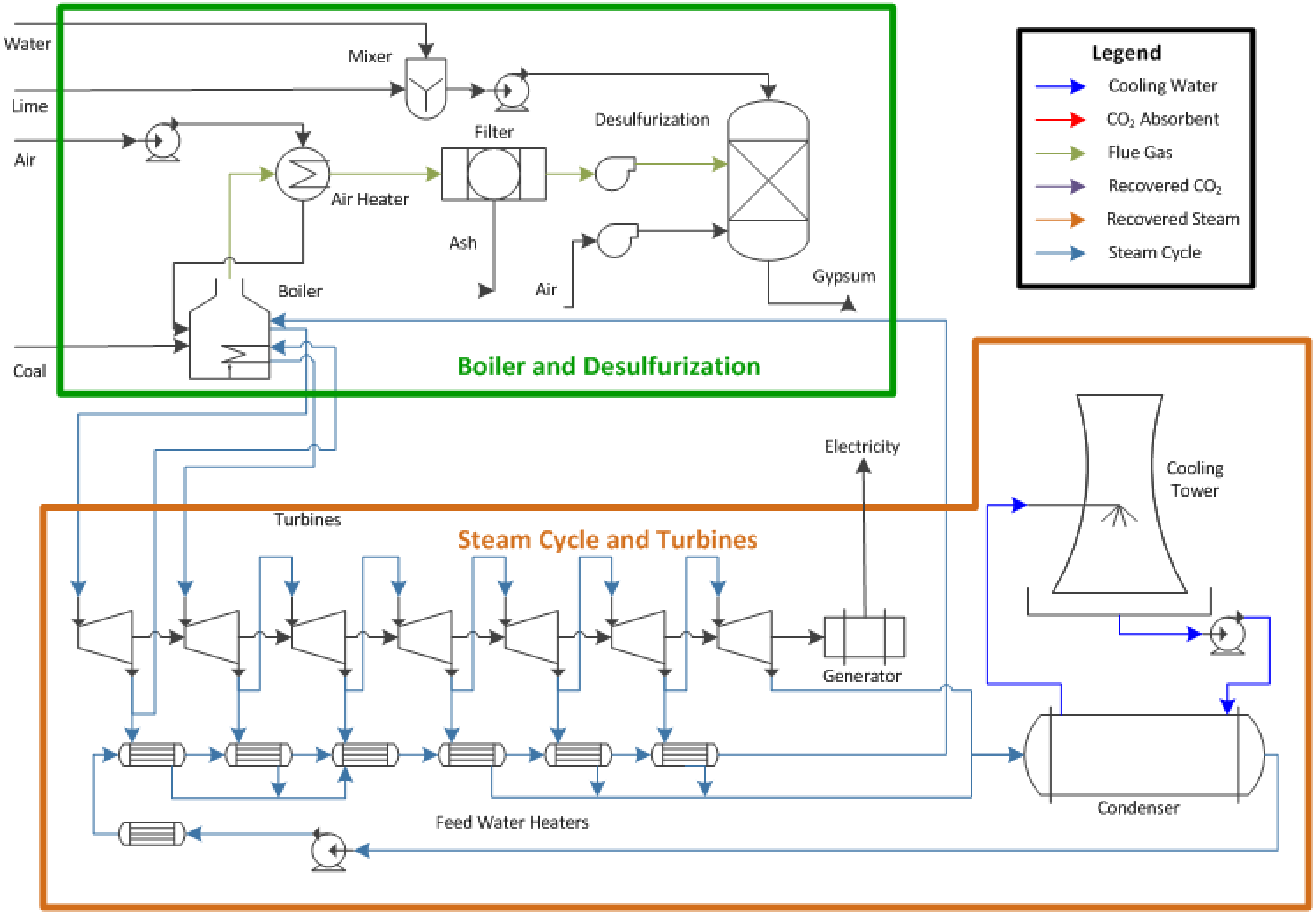
Pre-Combustion Carbon Capture Modules

- ***Physical absorption systems***
- *Chemical looping*
- ***Solid sorbents***
- ***Adsorption***
- *Membranes*
- *Ionic liquids*
- *Compression*

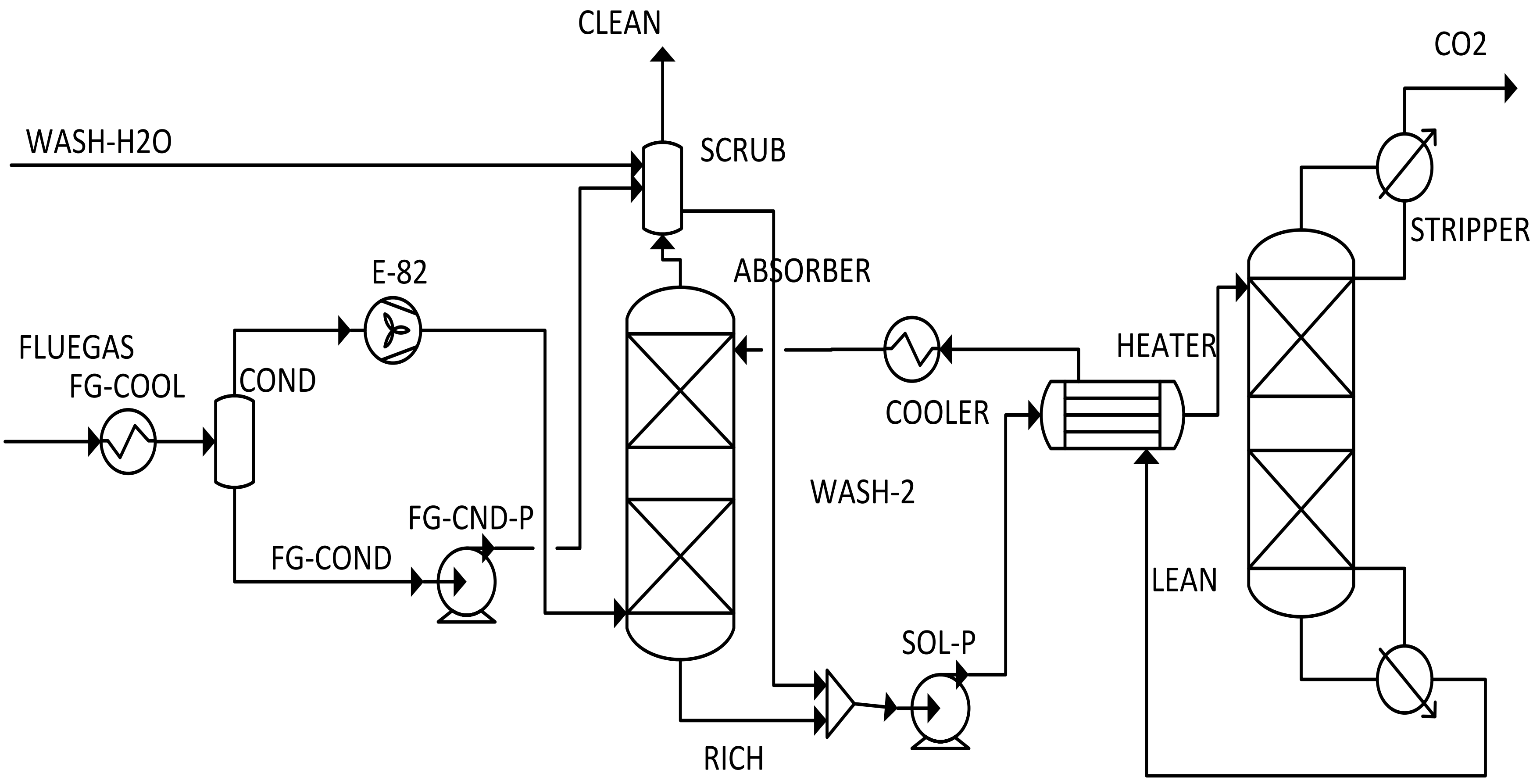
Plantwide Water Simulator

- *Cooling alternatives*
- ***High fidelity cooling tower models***
- ***Nontraditional water sources***
- *Water recovery*
- ***Water treatment***
- *Cooling water & process water*

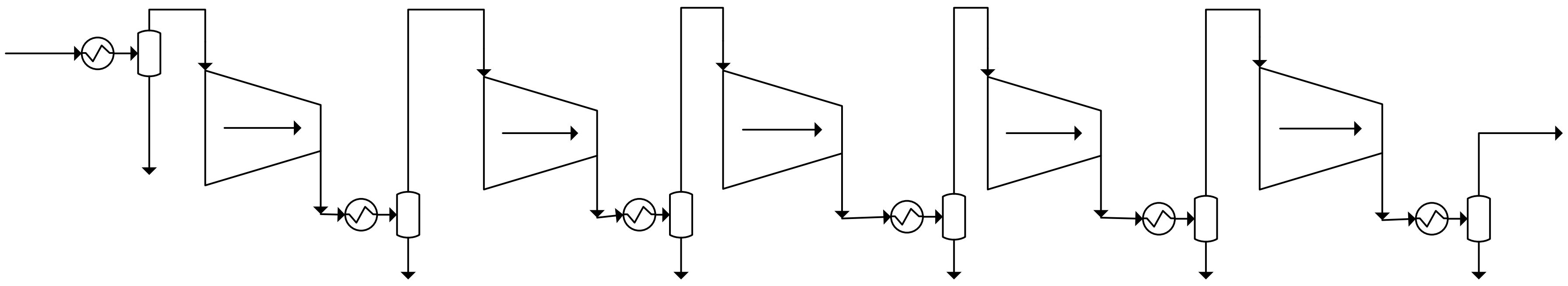
Subcritical PC Plant



MEA Module


CLEAN
CO2
WASH-H2O
SCRUB
STRIPPER
E-82
ABSORBER
FLUEGAS
FG-COOL
COND
HEATER
COOLER
WASH-2
FG-CND-P
FG-COND
LEAN
SOL-P
RICH

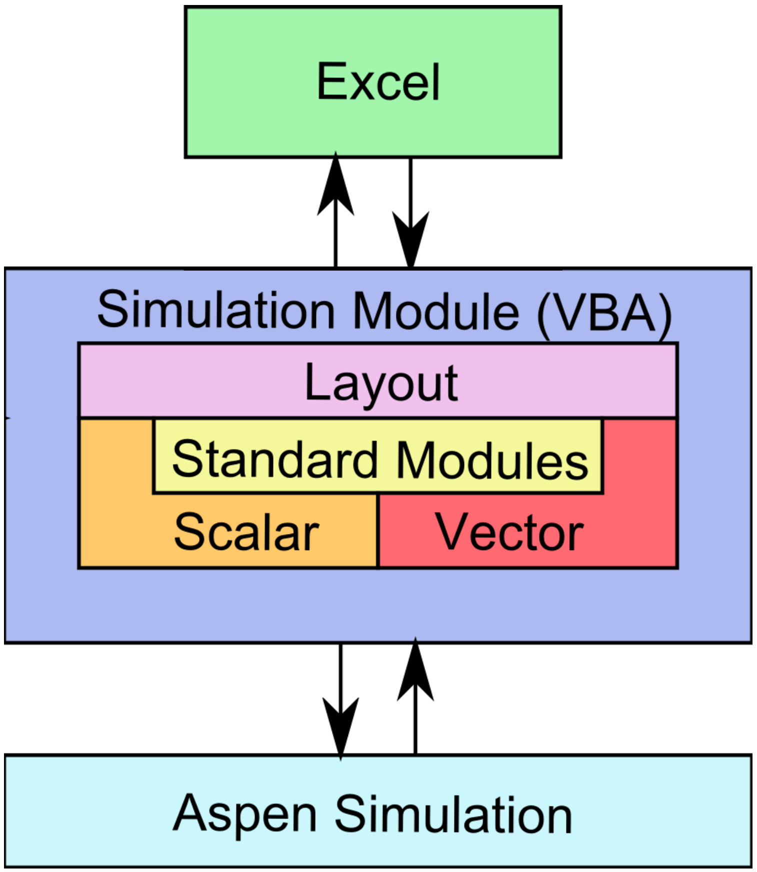
Compression



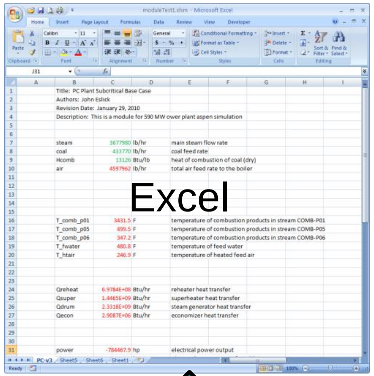
- 5 stage compression
- Intercoolers 265 F to variable T
- Water returned to process
- Final pressure 2200 psia

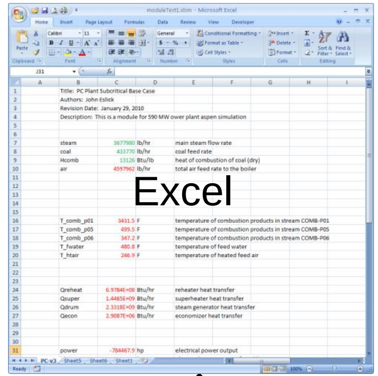
Simulation Interface

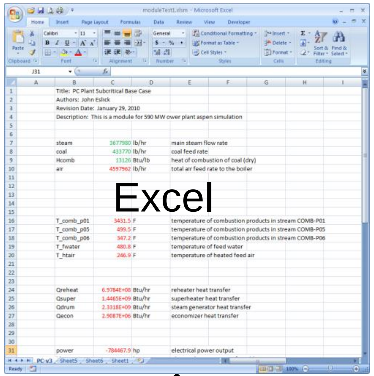
- Set simulation variables
- Supports structural changes
  - Feed stage
  - Number of stages
  - (not supported internally)
- Retrieves results
- Perform post-processing
  - Cost estimation
  - Objective function calculations



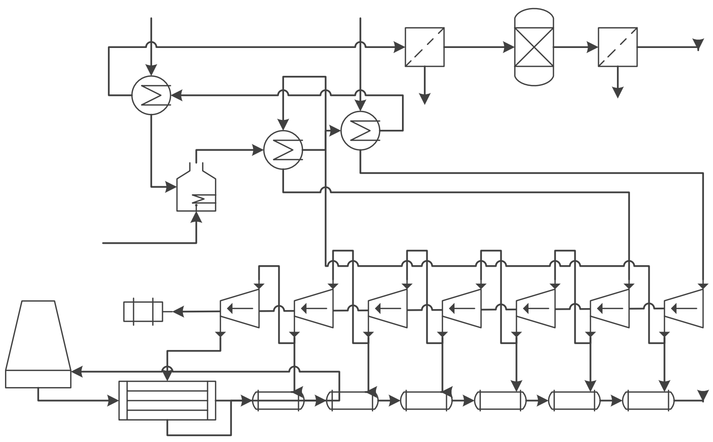
Modular Framework for Design and Optimization



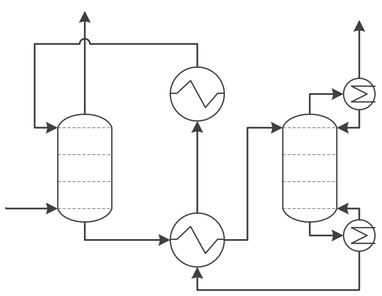




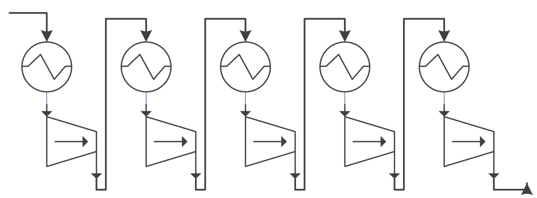
Power Plant Module



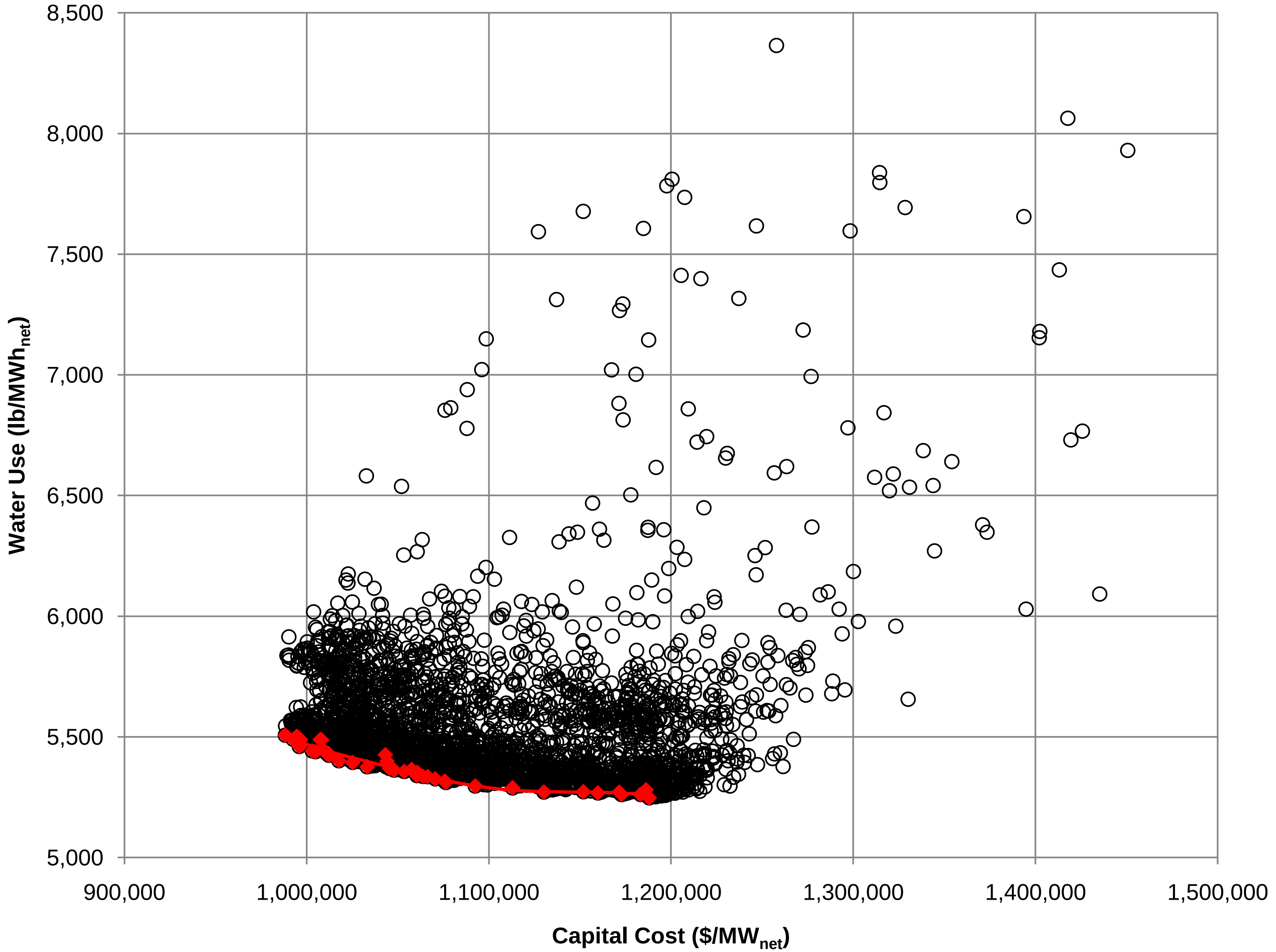
CO_2 Capture Module



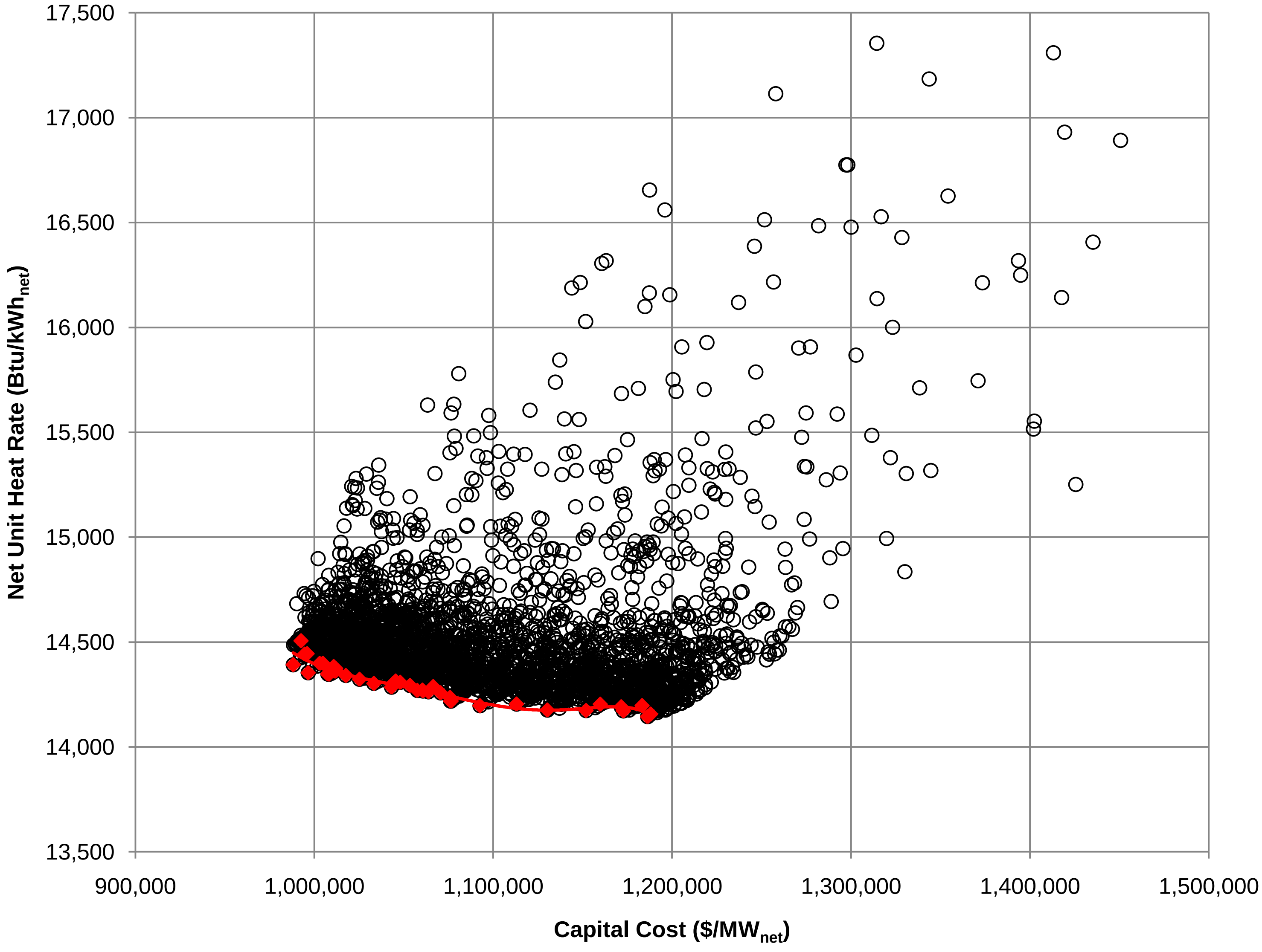
Compression Module



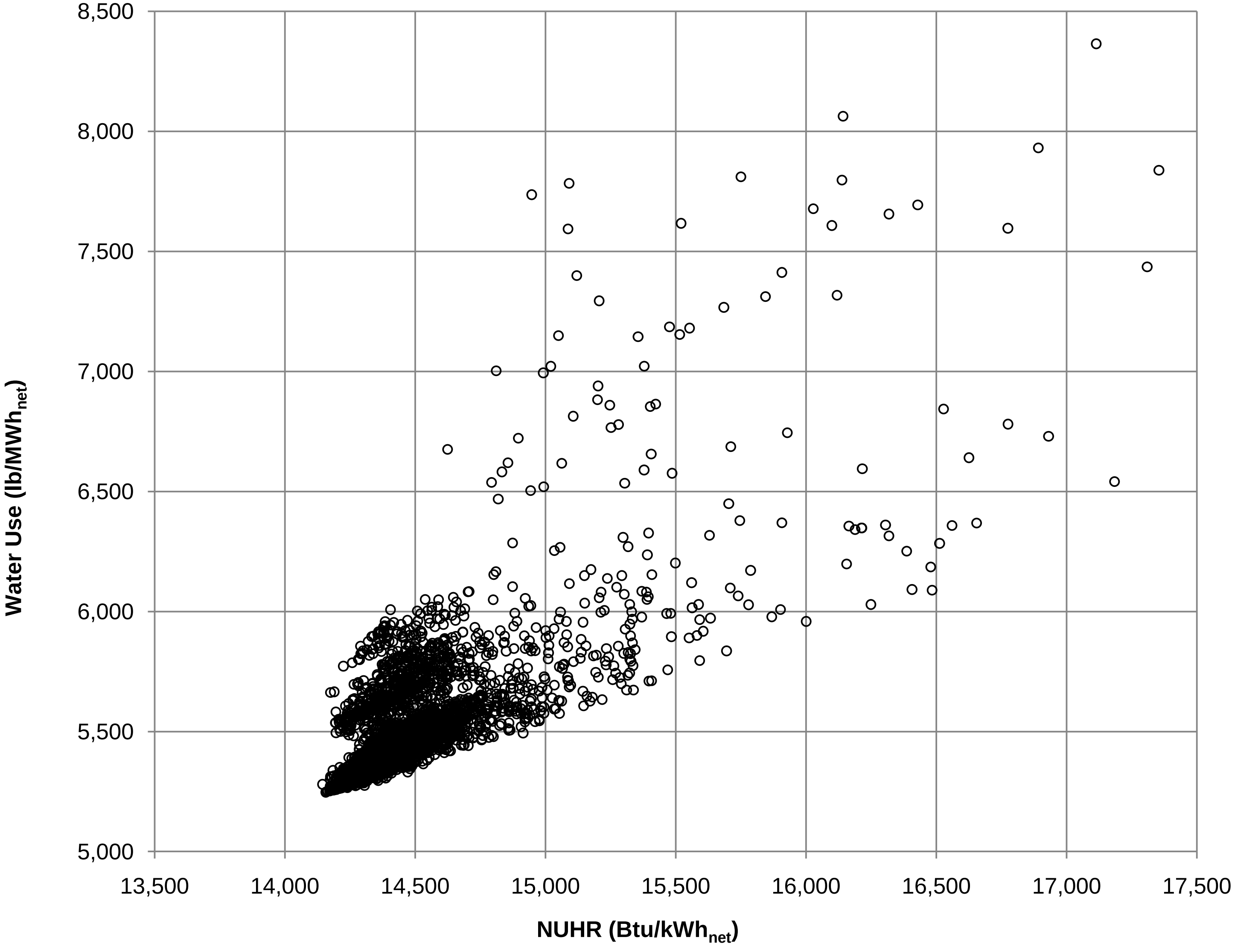
Capital Cost vs. Water Use



Capital Cost vs. NUHR



NUHR vs. Water Use

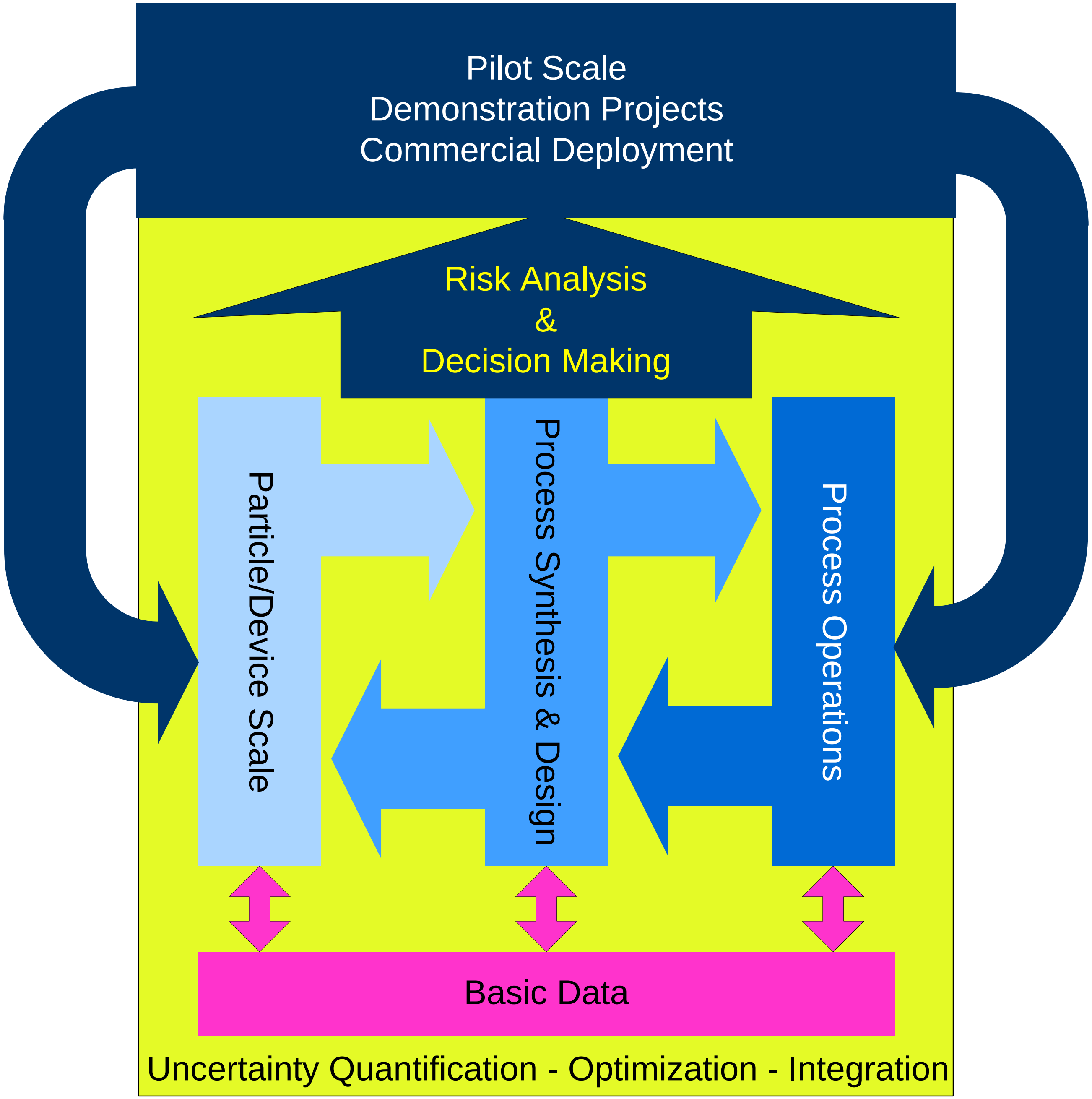


	Best Net Unit Heat Rate	Best Capital Cost	Best Water Use
NUHR (Btu/kWh)	14,145	14,392	14,157
Capital Cost ($/kW$_{net}$)	1,186	988	1,188
Overall Net Power Output (MW)	354.7	348.6	354.4
Total Capital Cost (Capture & Compression only)	$421 MM	$345 MM	$421 MM
Solvent Flow rate (gpm)	7,070	7,470	6,970
Lean Solvent Loading (mol CO_2/mol amine)	0.214	0.218	0.212
Rich Solvent Loading (mol CO_2/mol amine)	0.454	0.444	0.454
No. Absorber Stages	20	10	20
No. Stripper Stages	14	12	14
Cooling Water Evaporation (lb/MWh$_{net}$)	5,280	5,507	5,247

Optimized Process Systems

- Large potential improvement over initial design
- Essential for comparing technology
- Many non-intuitive interactions
- Understand competing objectives

Process Scale Up Tasks



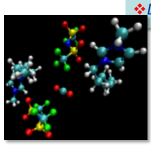
Carbon Capture Simulation Initiative

Ab initio QM
- *Energy, structure*
- *Charge, force field*
- *Interaction mechanisms*

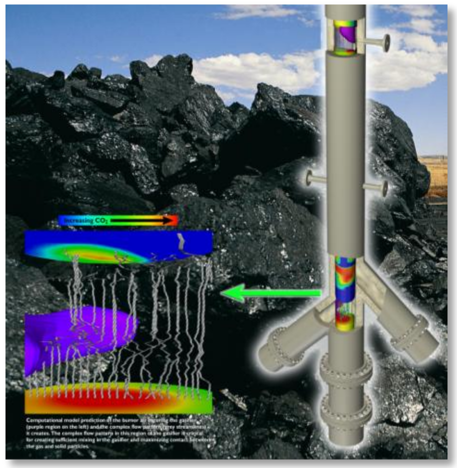
Monte Carlo
•Thermo dynamic Properties

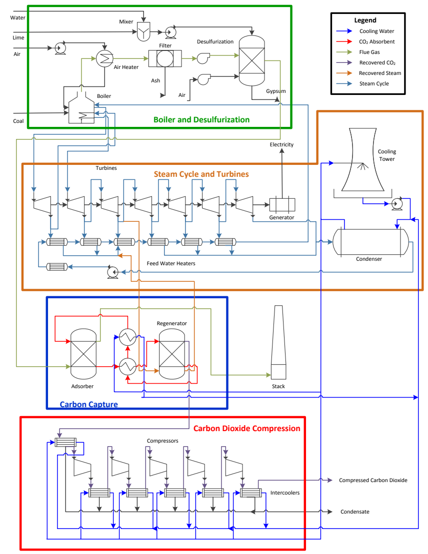
Molecular Dynamics
•Transport Properties

- *Search for better ILs*
- *Modify IL functionality*
- *Discover new IL*



A new ionic liquid that exhibits high CO_2 permeability and CO_2/H_2 selectivity was identified with this method.





Identify promising concepts and designs → *Develop optimal designs* → *Quantify technical risk in scale up*

Accelerate learning during development & deployment

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Modular Framework Research Team

- Optimization and computational infrastructure
  - ModeFrontier integration & multi-criteria, simulation-based optimization - NETL (Miller/Eslick)
  - Derivative-free “Blackbox” Optimization – CMU (Sahinidis/Cozad)
  - Surrogate model development – CMU (Sahinidis/Chang)
  - Simultaneous Superstructure-based Optimization – CMU (Grossmann/Yang)
  - Synthesis of Integrated IGCC Systems – CMU (Grossmann/Biegler/Kamath)
- Module development
  - Base plant modules
    - Predictive Plant Models (PC/IGCC) – NETL (Miller/Eslick)
    - Development of Predictive Turbine Models – NETL (Liese)
    - Oxycombustion Plant Model – NETL Albany (Summers/Oryshchyn/Harendra)
  - Carbon capture modules
    - Equilibrium & rate-based amine capture – NETL (Miller/Eslick)
    - Solid sorbent capture systems – NETL (Miller/Lee)
    - Membrane-based separation systems – NETL (Miller/Morinelly)
    - Compression system – NETL (Miller/Eslick)
    - Synthesis of Optimal PSA Cycles for CO2 Capture from Flue Gas – CMU (Biegler/Agarwal)
    - Synthesis of Optimal PSA Cycles for Hydrogen/CO2 Separation – CMU (Biegler/Vetukuri)
    - Cryogenic separation and hydrate-based separation – NETL (van Osdol)
  - Water-specific activities
    - Treated Municipal Wastewater for Power Plant Cooling – CMU (Dzombak/Hsieh)
    - Modeling Nontraditional Sources of Power Plant Water
      - IIT (Abbasian/Arastoopour/Walker/Safari/Strumendo)
    - Water from Oxycombustion – NETL Albany (Summers/Oryshchyn/Harendra)